Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 146 °C

Global applicability domain: Outside

Local applicability domain index: 1.69e-01

Confidence level: 4.25e-01

Nearest Neighbors from the Training Set

Image not found
Hexamethylmelamine
Measured: 173
Predicted: 154

Image not found
Dimorpholamine
Measured: 41.5
Predicted: 49.9

Image not found
Alfentanil
Measured: 141
Predicted: 136

Image not found
2-(1,3-Dimethylxanthinyl-7-methyl)-4-methylmorpholine
Measured: 177
Predicted: 154

Image not found
N,N-Dinitrosopentamethylenetetramine
Measured: 205
Predicted: 194